Measuring Conditional Dependence with Kernels

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Outline

1. Introduction

2. Characterization of conditional independence with kernels

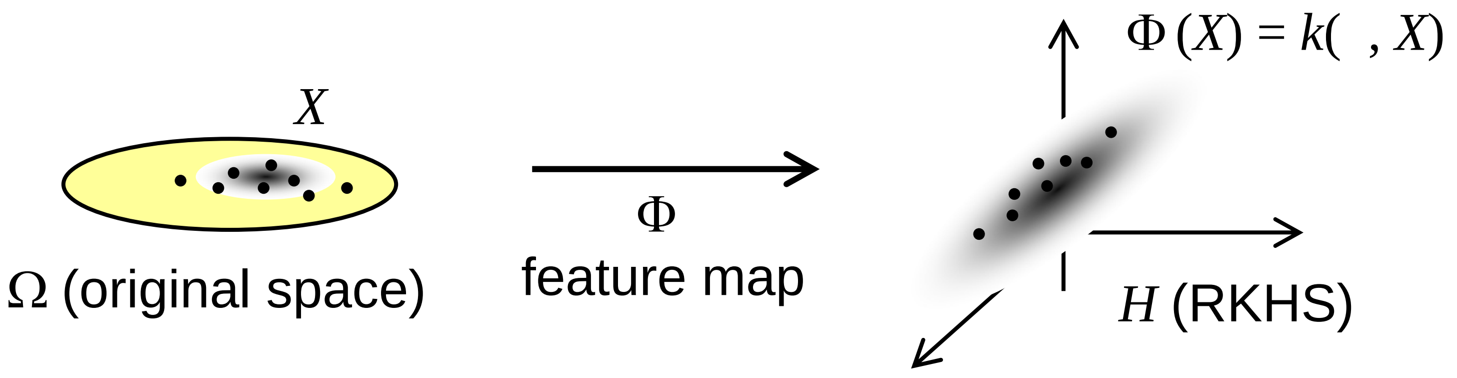
3. Conditional dependence measure with normalized operators and its kernel-free expression.

4. Experiments

5. Concluding remarks

Introduction

- "Kernel methods" for nonlinear relations
  - Positive definite kernels have been used for capturing nonlinearity of original data.   *e.g*. Support vector machine.
  - Kernelization: mapping data into a functional space (RKHS) and apply linear methods on RKHS.
  - Consider linear statistics (mean, variance, …) on RKHS, and their meaning on the original space.



- Representing probabilities
  - Determining probabilities (Arthur Gretton's talk)
  - Characterizing independence (Arthur Gretton's talk)
  - Characterizing conditional independence

- Motivation
  - Dependence among many variables
  - Conditional independence is essential for many probabilistic modeling
    e.g. graphical modeling

Positive Definite Kernel and RKHS

- Positive definite kernel (p.d. kernel)

Ω: set. $k:\Omega\times\Omega\to\mathbf{R}$

k is positive definite if $k(x,y) = k(y,x)$ and for any $n\in\mathbf{N}$, $x_1,\ldots x_n\in\Omega$ the matrix $\left(k(x_i,x_j)\right)_{i,j}$ (Gram matrix) is positive semidefinite.

  – Example: Gaussian RBF kernel $k(x,y)=\exp\left(-\|x-y\|^2/\sigma^2\right)$

- Reproducing kernel Hilbert space (RKHS)

k: p.d. kernel on Ω.

$\Rightarrow$ $\exists 1\ H$: reproducing kernel Hilbert space (RKHS)

1) $k(\cdot,x)\in H$ for all $x\in\Omega$.

2) $\mathrm{Span}\{k(\cdot,x)\mid x\in\Omega\}$ is dense in H.

3) $\langle k(\cdot,x), f\rangle_H = f(x)$ (reproducing property)

Functional data (feature map)

$$\Phi : \Omega \to H, \quad x \mapsto k(\cdot, x) \qquad i.e. \quad \Phi(x) = k(\cdot, x)$$

$$\langle \Phi(x), f \rangle = f(x)$$ (reproducing property)

Data: $X_1, \ldots, X_N$ → $\Phi_X(X_1), \ldots, \Phi_X(X_N)$: functional data

Why RKHS?

– By the reproducing property, computation of the inner product on RKHS does not need expansion by basis functions.

$$f(\cdot) = \sum_i a_i k(\cdot, x_i), \quad g(\cdot) = \sum_j b_j k(\cdot, x_j)$$

$$\Rightarrow \quad \langle f, g \rangle = \sum_{i,j} a_i b_j k(x_i, x_j)$$

Advantageous for high-dimensional data of small sample size.

Representing Nonlinear Dependence

- **Kernel Statistics: linear statistics on RKHS**

  X , Y : general random variables on Ω_X and Ω_Y , resp.

  Prepare RKHS (H_X, k_X) and (H_X , k_X) defined on Ω_X and Ω_Y, resp

  Define random variables on the RKHS H_X and H_Y by

$$\Phi_X(X) = k_X(\cdot, X) \qquad \Phi_Y(Y) = k_Y(\cdot, Y)$$

  – Covariance

$$\Sigma_{YX} \equiv E[(\Phi_Y(Y) - \mu_X)(\Phi_X(X) - \mu_Y)^T] \longrightarrow \Sigma_{XY} = O \Leftrightarrow X \perp\!\!\!\perp Y$$

  – Conditional covariance

$$\Sigma_{YX|Z} \equiv \Sigma_{YX} - \Sigma_{YZ}\Sigma_{ZZ}^{-1}\Sigma_{ZX} \longrightarrow \Sigma_{YX|Z} = O \Leftrightarrow X \perp\!\!\!\perp Y \mid Z$$

  – c.f. Gaussian variables

$$V_{XY} = O \Leftrightarrow X \perp\!\!\!\perp Y$$

$$V_{YX|Z} = O \Leftrightarrow X \perp\!\!\!\perp Y \mid Z$$

Richness Assumption on RKHS

k: kernel on a measurable space $(\Omega, \mathcal{B})$. H: associated RKHS.

Assumption (A):

$\exists q \geq 1.$ $H + \mathbf{R}$ is dense in $L^q(P)$ for any probability P on $(\Omega, \mathcal{B})$,

– RKHS can approximates various functions such as the index function of a measurable set, polynomials, and $e^{\sqrt{-1}\omega^T x}$.

– Example: Gaussian kernel on the entire $\mathbf{R}^m$

$$k_G(x, y) = \exp\left(-\frac{\|x - y\|^2}{2\sigma^2} \right)$$

Laplacian kernel on the entire $\mathbf{R}^m$

$$k_L(x, y) = \exp\left(-\lambda \sum_{i=1}^m |x_i - y_i| \right)$$

Covariance on RKHS

– Definition: cross-covariance operator

X , Y : general random variables on Ω_X and Ω_Y , resp.

Prepare RKHS (H_X, k_X) and (H_X , k_X) defined on Ω_X and Ω_Y, resp.

There is a unique operator $\Sigma_{YX} : H_X \to H_Y$ such that

$$\langle g, \Sigma_{YX} f \rangle = E[g(Y) f(X)] - E[g(Y)]E[f(X)] \quad (= \mathrm{Cov}[f(X), g(Y)])$$

for all $f \in H_X, g \in H_Y$

– Independence by cross-covariance operator

Under (A),

X and Y are independent $\Leftrightarrow$ $\Sigma_{XY} = O$

$$E[g(Y) f(X)] = E[g(Y)]E[f(X)]$$

- *c.f.* Characteristic function

$$X \perp\!\!\!\perp Y \quad \Leftrightarrow \quad E_{XY}[e^{\sqrt{-1}(uX+vY)}] = E_X[e^{\sqrt{-1}uX}]E_Y[e^{\sqrt{-1}vY}]$$

Conditional Covariance on RKHS

- Conditional Cross-covariance operator

  X, Y, Z : random variables on $\Omega_X, \Omega_Y, \Omega_Z$ (resp.).

  $(H_X, k_X), (H_Y, k_Y), (H_Z, k_Z)$: RKHS defined on $\Omega_X, \Omega_Y, \Omega_Z$ (resp.).

  – Conditional cross-covariance operator $H_X \to H_Y$

$$\Sigma_{YX|Z} \equiv \Sigma_{YX} - \Sigma_{YZ}\Sigma_{ZZ}^{-1}\Sigma_{ZX}$$

  – Conditional covariance operator

$$\Sigma_{YY|Z} \equiv \Sigma_{YY} - \Sigma_{YZ}\Sigma_{ZZ}^{-1}\Sigma_{ZY}$$

  – Note: Σ_{ZZ}^{-1} may not exist. But, we have the decomposition

$$\Sigma_{YX} = \Sigma_{YY}^{1/2} W_{YX} \Sigma_{XX}^{1/2} \qquad \text{with operator norm } \|W_{YX}\| \le 1$$

  Rigorously, define $\Sigma_{YX|Z} \equiv \Sigma_{YX} - \Sigma_{YY}^{1/2} W_{YZ} W_{ZX} \Sigma_{XX}^{1/2}$

Relation with regression error

Theorem (FBJ'06)

Y, Z : random variables on Ω_Y, Ω_Z (resp.).

(H_Y, k_Y), (H_Z, k_Z) : RKHS defined on Ω_Y, Ω_Z (resp.).

$$\langle g, \Sigma_{YY|Z} g \rangle = \inf_{f \in H_Z} E\left| \left(g(Y) - E[g(Y)] \right) - \left(f(Z) - E[f(Z)] \right) \right|^2$$

$$= \inf_{f \in H_Z} Var\left[g(Y) - f(Z) \right] \qquad (\forall g \in H_Y)$$

c.f. for Gaussian variables,

$$b^T V_{YY|Z} b = \min_a \left| b^T \tilde{Y} - a^T \tilde{Z} \right|^2 \qquad (\tilde{Y} = Y - E[Y], \tilde{Z} = Z - E[Z])$$

Residual error of linear regression is given by the conditional covariance matrix.

– Rough sketch of the proof

$$E\left|\left(g(Y)-E[g(Y)]\right)-\left(f(Z)-E[f(Z)]\right)\right|^2$$

$$=\langle f,\Sigma_{ZZ}f\rangle-2\langle f,\Sigma_{ZY}g\rangle+\langle g,\Sigma_{YY}g\rangle$$

$$=\left\|\Sigma_{ZZ}^{1/2}f\right\|^2-2\left\langle f,\Sigma_{ZZ}^{1/2}W_{ZY}\Sigma_{YY}^{1/2}g\right\rangle+\left\|\Sigma_{YY}^{1/2}g\right\|^2$$

$$=\left\|\Sigma_{ZZ}^{1/2}f-W_{ZY}\Sigma_{YY}^{1/2}g\right\|^2+\left\|\Sigma_{YY}^{1/2}g\right\|^2-\left\|W_{ZY}\Sigma_{YY}^{1/2}g\right\|^2$$

$$=\underline{\left\|\Sigma_{ZZ}^{1/2}f-W_{ZY}\Sigma_{YY}^{1/2}g\right\|^2}+\left\langle g,\left(\Sigma_{YY}-\Sigma_{YY}^{1/2}W_{YZ}W_{ZY}\Sigma_{YY}^{1/2}\right)g\right\rangle$$

This part can be arbitrary small
by choosing *f*.

Relation with conditional covariance

Theorem (FBJ'06, Sun et al. '07)

X, Y, Z : random variables on Ω_X, Ω_Y, Ω_Z (resp.).

(H_X, k_X), (H_Y, k_Y), (H_Z, k_Z) : RKHS defined on Ω_X, Ω_Y, Ω_Z (resp.).

Assume

$$H_Z + \mathbf{R} \text{ : dense in } L^2(P_Z)$$

then,

$$\langle g, \Sigma_{YX|Z} f \rangle = E\big[Cov[g(Y), f(X) \mid Z]\big] \qquad (\forall f \in H_X, g \in H_Y)$$

– *c.f.* for Gaussian variable

$$a^T V_{XY|Z} b = Cov[a^T X, b^T Y \mid Z]$$

(not dependent on the value of z)

– Sketch of the proof for the simpler case of $X = Y$ and $f = g$,

i.e. $\langle g, \Sigma_{YY|Z} g \rangle = E\left[Var[g(Y) \mid Z] \right]$

Lemma $Var[Y] = Var_X\left[E_{Y|X}[Y \mid X] \right] + E_X\left[Var_{Y|X}[Y \mid X] \right]$

$$\langle g, \Sigma_{YY|Z} g \rangle = \inf_{f \in H_Z} Var\left[g(Y) - f(Z) \right]$$

$$= \inf_{f \in H_Z} \left\{ Var\left[E\left[g(Y) - f(Z) \mid Z \right] \right] + E\left[Var\left[g(Y) - \underbrace{f(Z)}_{\text{const.}} \mid \underline{Z} \right] \right] \right\}$$

$$= \inf_{f \in H_Z} Var\left[\underbrace{E\left[g(Y) \mid Z \right]}_{\in L^2(P_Z)} - f(Z) \right] + E\left[Var\left[g(Y) \mid Z \right] \right]$$

$$= 0 + E\left[Var\left[g(Y) \mid Z \right] \right]$$ (by denseness assumption)

Conditional Independence

<u>Theorem (FBJ04, Sun et al 07)</u>

Under (A),

$$\Sigma_{YX|Z} = O \quad \Leftrightarrow \quad P_{YX} = E_Z\left[P_{Y|Z} \otimes P_{X|Z}\right]$$

where $E_Z\left[P_{Y|Z} \otimes P_{X|Z}\right]$ is a probability on $\Omega_X \times \Omega_Y$ defined by

$$E_Z\left[P_{Y|Z} \otimes P_{X|Z}\right](B \times A) = \int P_{Y|Z}(B \mid Z = z) P_{X|Z}(A \mid Z = z) dP_Z(z)$$

With p.d.f.

$$E_Z\left[P_{Y|Z} \otimes P_{X|Z}\right](A \times B) = \int \int_A p_{X|Z}(x \mid z) d\mu_1(x) \int_B p_{Y|Z}(y \mid z) d\mu_2(y) dP_Z(z)$$

Remark: The assertion $P_{YX} = E_Z\left[P_{Y|Z} \otimes P_{X|Z}\right]$ is weaker than the conditional independence $P_{YX|Z} = P_{Y|Z} \otimes P_{X|Z}$

c.f. for Gaussian variables

$$V_{YX|Z} = O \quad \Leftrightarrow \quad X \perp\!\!\!\perp Y \mid Z$$

– Proof of $\Sigma_{YX|Z} = O \quad \Rightarrow \quad P_{YX} = E_Z\left[P_{Y|Z} \otimes P_{X|Z}\right]$

$\Sigma_{YX|Z} = O$ means $E\left[Cov[g(Y), f(X) \mid Z]\right] = 0$

$$\Rightarrow \quad E\left[E[g(Y)f(X) \mid Z]\right] = E\left[E[g(Y) \mid Z]E[f(X) \mid Z]\right]$$

$$\Rightarrow \quad E_{P_{XY}}[g(Y)f(X)] = E_{E_Z[P_{Y|Z} \otimes P_{X|Z}]}[g(Y)f(X)] \qquad \forall f \in H_X, g \in H_Y$$

Under (A), by approximating the index function $I_{A \times B}(x, y)$

$$P_{YX} = E_Z\left[P_{Y|Z} \otimes P_{X|Z}\right]$$

Characterization of conditional independence

<u>Theorem</u>

Define the augmented variable $\tilde{X} = (X, Z)$ and define a kernel on $\Omega_X \times \Omega_Z$ by

$$k_{\tilde{X}} = k_X k_Z$$

Under (A),

$$\Sigma_{Y\tilde{X}|Z} = O \quad \Leftrightarrow \quad X \perp\!\!\!\perp Y \mid Z$$

$$\Sigma_{Y\tilde{X}|Z} = O \quad \Leftrightarrow \quad \Sigma_{\tilde{Y}X|Z} = O \quad \Leftrightarrow \quad \Sigma_{\tilde{Y}\tilde{X}|Z} = O \quad \Leftrightarrow \quad X \perp\!\!\!\perp Y \mid Z$$

proof)

$$\Sigma_{Y[X,Z]|Z} = O \quad \Rightarrow \quad p(x, y, z') = \int p(x, z' \mid z) p(y \mid z) p(z) dz$$

where $p(x, z' \mid z) = p(x \mid z) \delta(z' - z)$

$$\Rightarrow \qquad p(x, y, z') = p(x \mid z') p(y \mid z') p(z')$$

i.e. $\quad p(x, y \mid z') = p(x \mid z') p(y \mid z')$

Normalized Cond. Covariance

- Normalized conditional cross-covariance operator

Definition

$$W_{YX|Z} = \Sigma_{YY}^{-1/2}\Sigma_{YX|Z}\Sigma_{XX}^{-1/2} = \Sigma_{YY}^{-1/2}\left(\Sigma_{YX} - \Sigma_{YZ}\Sigma_{ZZ}^{-1}\Sigma_{ZX}\right)\Sigma_{XX}^{-1/2}$$

More rigorously,

$$W_{YX|Z} \equiv W_{YX} - W_{YZ}W_{ZX}$$

Recall: $\Sigma_{YX} = \Sigma_{YY}^{1/2}W_{YX}\Sigma_{XX}^{1/2}$

– Conditional independence

Under the assumption (A),

$$W_{Y\tilde{X}|Z} = O \quad \Leftrightarrow \quad X \perp\!\!\!\perp Y \mid Z$$

Conditional Dependence Measure

– HS Normalized Conditional Independence Criteria

$$HSNCIC = \left\| W_{\tilde{X}\tilde{Y}|Z} \right\|_{HS}^{2}$$

$$HSNCIC = 0 \qquad \Leftrightarrow \qquad X \perp\!\!\!\perp Y \mid Z$$

– Hilbert-Schmidt norm of an operator

$A : H_1 \to H_2$ operator on a Hilbert space

A is called Hilbert-Schmidt if for complete orthonormal systems $\{\varphi_i\}$ of H_1 and $\{\psi_j\}$ of H_2

$$\sum_j \sum_i \langle \psi_j, A\varphi_i \rangle^2 < \infty.$$

Hilbert-Schmidt norm is defined by

$$\|A\|_{HS}^2 = \sum_j \sum_i \langle \psi_j, A\varphi_i \rangle^2$$

c.f. Frobenius norm of a matrix

Kernel-free Expression

<u>Theorem</u>

Assume

P_{XY} and $E_Z\left[P_{Y|Z} \otimes P_{X|Z}\right]$ have density $p_{XY}(x,y)$ and $p_{X\perp Y|Z}(x,y)$, resp.

$H_Z + \mathbf{R}$ and $H_X \otimes H_Y + \mathbf{R}$ are dense in $L^2(P_Z)$ and $L^2(P_X \otimes P_Y)$, resp.

W_{YX} and $W_{YZ} W_{ZX}$ are Hilbert-Schmidt.

Then,

$$\| W_{YX|Z} \|_{HS}^2 = \iint \left(\frac{p_{XY}(x,y) - p_{X\perp Y|Z}(x,y)}{p_X(x) p_Y(y)} \right)^2 p_X(x) p_Y(y) dx dy$$

In the special case of $Z = \phi$

$$\| W_{YX} \|_{HS}^2 = \iint \left(\frac{p_{XY}(x,y)}{p_X(x) p_Y(y)} - 1 \right)^2 p_X(x) p_Y(y) dx dy$$

- Kernel-free expression, though the definitions are given by kernels!

– Kernel-free value is reasonable as a “measure” of dependence. *c.f.* If unnormalized operators are used, the measures do depend on the choice of kernel (HSIC, Gretton et al. ALT2005)

– In the unconditional case,

$$\text{HS-NIC} = \| W_{YX} \|_{HS}^2$$

is equal to the mean square contingency, which is one of the popular measures of dependence.

– In the conditional case, if we use the augmented variables

$$\| W_{\tilde{Y}\tilde{X}|Z} \|_{HS}^2$$
$$= \iint \left(\frac{p_{XYZ}(x,y,z) - p_{X|Z}(x|z)\, p_{Y|Z}(y|z)\, p_Z(z)}{p_{XZ}(x,z)\, p_{YZ}(y,z)} \right)^2 p_{XZ}(x,z)\, p_{YZ}(y,z)\, dx dy dz$$

(conditional mean square contingency)

– Key idea of the proof

By the eigendecomposition of Σ_{XX} and Σ_{YY} , we have CONS $\{\varphi_i\}$ of H_X and $\{\psi_j\}$ of H_Y such that

$$\Sigma_{XX}\varphi_i = \lambda_i \varphi_i, \quad \Sigma_{YY}\psi_j = \nu_j \psi_j \qquad (\lambda_i \ge 0, \nu_j \ge 0)$$

Define

$$\tilde{\varphi}_i = \frac{\varphi_i - E[\varphi_i]}{\sqrt{\lambda_i}}, \quad \tilde{\psi}_j = \frac{\psi_j - E[\psi_j]}{\sqrt{\nu_i}}$$

By the denseness assumption, $\{1\} \bigcup \{\tilde{\varphi}_i \tilde{\psi}_j\}_{i,j}$ is CONS of $L^2(P_X \otimes P_Y)$

$$\sum_{i,j} \left\langle \psi_j, W_{YX}\varphi_i \right\rangle^2 = \sum_{i,j} \left\langle \Sigma_{YY}^{-1/2}\psi_j, \Sigma_{YX}\Sigma_{XX}^{-1/2}\varphi_i \right\rangle^2 = \sum_{i,j} \left\langle \frac{\psi_j}{\sqrt{\nu_j}}, \Sigma_{YX}\frac{\varphi_i}{\sqrt{\lambda_i}} \right\rangle^2$$

$$= \sum_{i,j} E_{XY}\left[\tilde{\psi}_j(Y)\tilde{\varphi}_i(X)\right]^2 = \sum_{i,j} \left(\tilde{\psi}_j(Y)\tilde{\varphi}_i(X), \frac{p_{XY}}{p_X p_Y} \right)^2_{L^2(P_X \otimes P_Y)}$$

$$= \left\| \frac{p_{XY}}{p_X p_Y} \right\|^2_{L^2(P_X \otimes P_Y)} - 1$$

etc.

Empirical Measures

- Empirical estimation is straightforward with the kernel method.
- Inversion → regularization: $\Sigma_{XX}^{-1} \quad \to \quad (\Sigma_{XX} + \varepsilon I)^{-1}$
- Replace the covariances in $W_{YX} = \Sigma_{YY}^{-1/2}\Sigma_{YX}\Sigma_{XX}^{-1/2}$ by the empirical ones given by the data $\Phi_X(X_1),\ldots,\ \Phi_X(X_N)$ and $\Phi_Y(Y_1),\ldots,\ \Phi_Y(Y_N)$

$$HSNIC_{emp} = \mathrm{Tr}\left[R_X R_Y\right]$$ (dependence measure)

$$HSNCIC_{emp} = \mathrm{Tr}\left[R_{\ddot{X}} R_{\ddot{Y}} - 2R_{\ddot{X}} R_{\ddot{Y}} R_Z + R_{\ddot{X}} R_Z R_{\ddot{Y}} R_Z\right]$$

(conditional dependence measure)

where $R_{\ddot{X}} \equiv G_{\ddot{X}}\left(G_{\ddot{X}} + N\varepsilon_N I_N\right)^{-1}$ etc.

- $\text{HSNIC}_{\text{emp}}$ and $\text{HSNCIC}_{\text{emp}}$ give kernel estimates for the mean square contingency and conditional mean square contingency, resp.

Relation with Other Measures

- Mutual Information

$$MI(X,Y) = \iint p_{XY}(x,y)\log\frac{p_{XY}(x,y)}{p_X(x)p_Y(y)}\,d\mu_X(x)d\mu_Y(y)$$

- MI and HSNIC

$$\boxed{HSNIC(X,Y) \le MI(X,Y)}$$

$\because$)

$$\begin{aligned} HSNIC &= \iint p_{XY}(x,y)\left(\frac{p_{XY}(x,y)}{p_X(x)p_Y(y)} - 1\right)d\mu_1(x)d\mu_2(y) \\ &\le \iint p_{XY}(x,y)\log\frac{p_{XY}(x,y)}{p_X(x)p_Y(y)}\,d\mu_1(x)d\mu_2(y) \quad = MI \end{aligned}$$

$$(\log z \le z - 1)$$

– Mutual Information:
  - Information-theoretic meaning.
  - Estimation is not straightforward for continuous variables. Explicit estimation of p.d.f. is difficult for high-dimensional data.
    – Parzen-window is sensitive to the band-width.
    – Partitioning may cause a large number of bins.
  - Some advanced methods: e.g. k-NN approach (Kraskov et al. 2004, Ku&Fine 2005).

– Kernel method:
  - Explicit estimation of p.d.f. is not required;

    the dimension of data does not appear explicitly, but it is influential in practice.
  - Kernel / kernel parameters must be chosen.

Statistical Consistency

Theorem (FGSS2007)

Assume that $W_{YX|Z}$ is Hilbert-Schmidt, and the regularization coefficient satisfies

$$\varepsilon_N \to 0 \qquad N^{1/3}\varepsilon_N \to \infty.$$

Then,

$$\left\| \hat{W}_{YX|Z}^{(N)} - W_{YX|Z} \right\|_{HS} \to 0 \qquad (N \to \infty)$$

In particular,

$$\left\| \hat{W}_{YX|Z}^{(N)} \right\|_{HS} \to \left\| W_{YX|Z} \right\|_{HS} \qquad (N \to \infty)$$

i.e. $\mathrm{HSNCIC}_{\mathrm{emp}}$ ($\mathrm{HSNIC}_{\mathrm{emp}}$) converges to the population value HSNCIC (HSNIC, resp).

Choice of Kernel

- How to choose a kernel?
  - Empirical estimates still depend on the choice of kernels.
  - For unsupervised problems, such as independence measures, there are no theoretically reasonable methods.

  - Some heuristic methods which work:
    - Heuristics for Gaussian kernels

$$\sigma = \mathrm{median}\left\{ \left\| X_i - X_j \right\| \ | \ i \neq j \right\}$$

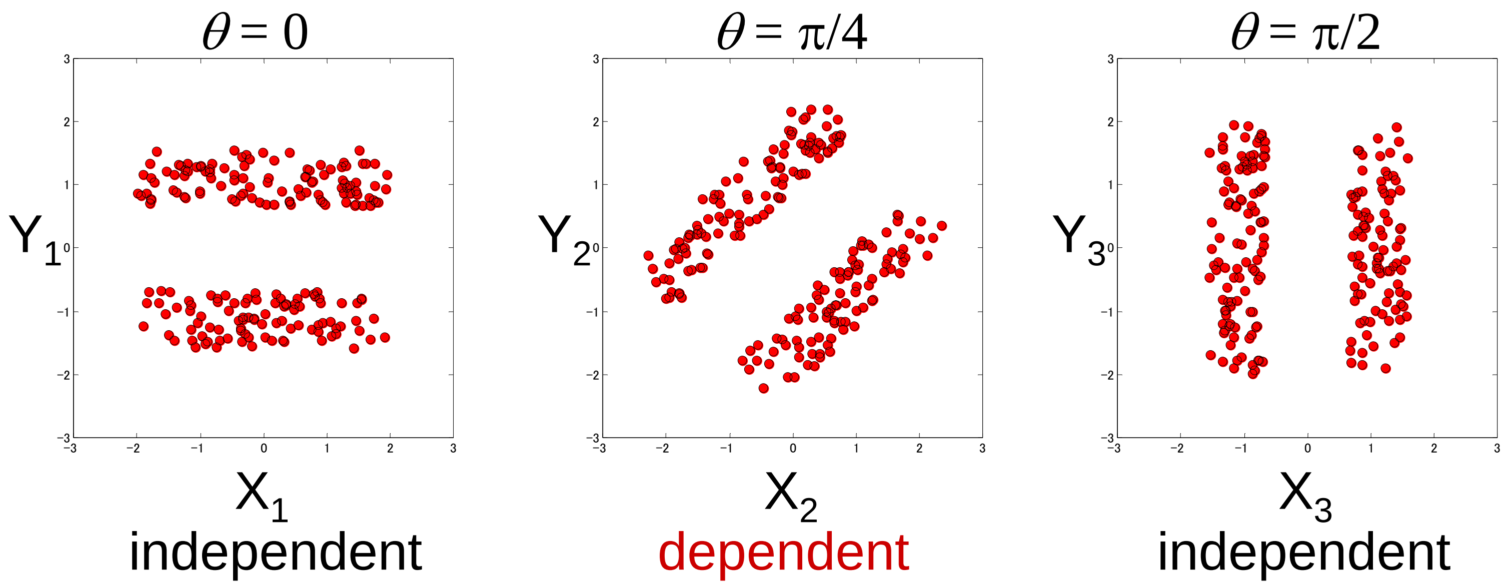
    - Speed of asymptotic convergence

$$\lim_{N \to \infty} Var\left[N \times HSNIC_{emp}^{(N)} \right] = 2 \left\| \Sigma_{XX} \right\|_{HS}^2 \left\| \Sigma_{YY} \right\|_{HS}^2 \quad \text{under independence}$$

Compare the bootstrapped variance and the theoretical one, and choose the parameter to give the minimum discrepancy.

Application to Independence Test

- Toy example



They are all uncorrelated, but dependent for $0 < \theta < \pi/2$

N = 200.
Permutation test is used.

indep. → more dependent

Angle	0.0	4.5	9.0	13.5	18.0	22.5
HSIC (Median)	93	92	63	5	0	0
HSIC (Asymp. Var.)	93	44	1	0	0	0
HSNIC ($\varepsilon = 10^4$, Median)	94	**23**	**0**	**0**	**0**	**0**
HSNIC ($\varepsilon = 10^6$, Median)	92	**20**	**1**	**0**	**0**	**0**
HSNIC ($\varepsilon = 10^8$, Median)	93	**15**	**0**	**0**	**0**	**0**
HSNIC (Asymp. Var.)	94	**11**	**0**	**0**	**0**	**0**
MI (#NN = 1)	93	62	11	0	0	0
MI (#NN = 3)	96	43	0	0	0	0
MI (#NN = 5)	97	49	0	0	0	0

acceptance of independence out of 100 tests (significance level = 5%)

Cond. Independence Test

- Permutation test with the kernel measure

$$T_N = \left\| \hat{\Sigma}_{YX|Z}^{(N)} \right\|_{HS}^2 \qquad \text{or} \qquad T_N = \left\| \hat{W}_{YX|Z}^{(N)} \right\|_{HS}^2$$

– If Z takes values in a finite set $\{1, \ldots, L\}$,

set $A_\ell = \{i \mid Z_i = \ell\} \ (\ell = 1, \ldots, L)$,

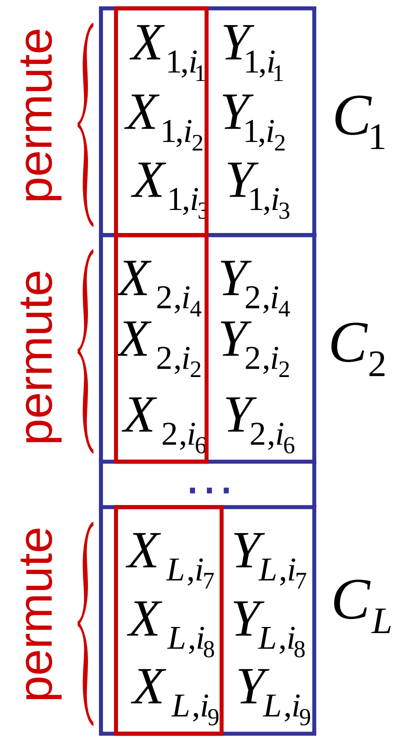
otherwise, partition the values of Z into L subsets $C_1, \ldots, C_L$, and set

$$A_\ell = \{i \mid Z_i \in C_\ell\} \quad (\ell = 1, \ldots, L).$$

– Repeat the following process B times: ($b = 1, \ldots, B$)

1. Generate pseudo cond. independent data $D^{(b)}$ by permuting X data within each A_ℓ.
2. Compute $T_N^{(b)}$ for the data $D^{(b)}$.

$\longrightarrow$ Approximate null distribution under cond. indep. assumption



– Set the threshold by the $(1-\alpha)$-percentile of the empirical distributions of $T_N^{(b)}$.

Kernel Method for Causality of Time Series

Causality by conditional independence

– Nonlinear extension of Granger causality

X is NOT a cause of Y if

$$p(Y_t \mid Y_{t-1},\ldots,Y_{t-p}, X_{t-1},\ldots,X_{t-p}) = p(Y_t \mid Y_{t-1},\ldots,Y_{t-p})$$

$\Leftrightarrow$

$$Y_t \perp\!\!\!\perp X_{t-1},\ldots,X_{t-p} \mid Y_{t-1},\ldots,Y_{t-p}$$

– Kernel measures for causality

$$HSNCIC = \left\| \hat{W}^{(N-p+1)}_{\tilde{Y}\mathbf{X_p}|\mathbf{Y_p}} \right\|^2_{HS}$$

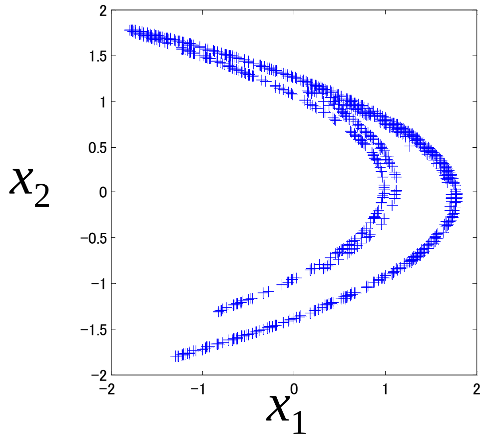
$$\mathbf{X}_{\mathrm{p}} = \{(X_{t-1,} X_{t-2}, \cdots, X_{t-p}) \in \mathbf{R}^p \mid t = p+1,\ldots,N\}$$
$$\mathbf{Y}_{\mathrm{p}} = \{(Y_{t-1,} Y_{t-2}, \cdots, Y_{t-p}) \in \mathbf{R}^p \mid t = p+1,\ldots,N\}$$

Example: Causality of Time-Series

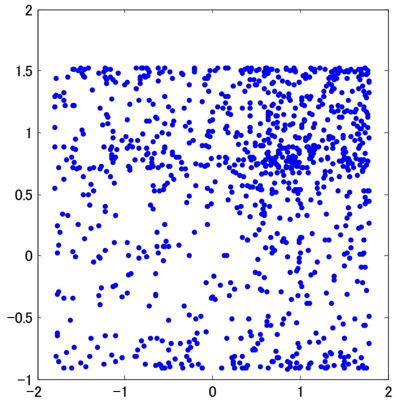
- Coupled Hénon map
  - X, Y:

$$\begin{cases} x_1(t+1) = 1.4 - x_1(t)^2 + 0.3x_2(t) \\ x_2(t+1) = x_1(t) \end{cases}$$

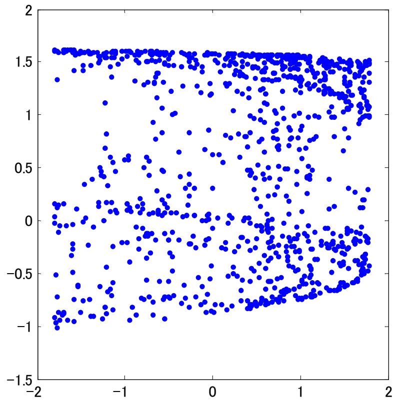
$$\begin{cases} y_1(t+1) = 1.4 - \left\{\underline{\gamma x_1(t)} y_1(t) + (1-\gamma) y_1(t)^2\right\} + 0.1y_2(t) \\ y_2(t+1) = y_1(t) \end{cases}$$



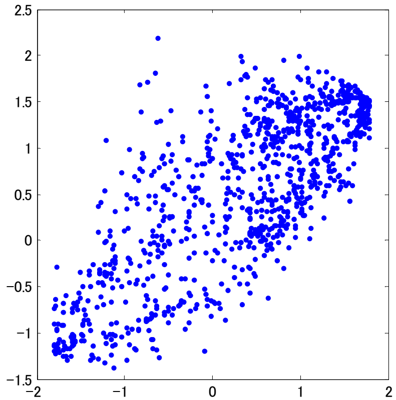
x_1-y_1



$\gamma = 0$



$\gamma = 0.25$



$\gamma = 0.8$

■ Causality of coupled Hénon map

- X is a cause of Y if $\gamma > 0$. $$Y_t \not\perp\!\!\!\perp X_{t-1},\dots,X_{t-p} \mid Y_{t-1},\dots,Y_{t-p}$$
- Y is not a cause of X for all γ. $$X_t \perp\!\!\!\perp Y_{t-1},\dots,Y_{t-p} \mid X_{t-1},\dots,X_{t-p}$$
- Permutation tests for non-causality with $HSNCIC = \left\| \hat{W}^{(N-p+1)}_{\ddot{Y}\mathbf{X_p}|\mathbf{Y_p}} \right\|^2_{HS}$

N = 100

$x_1 - y_1$	H$_0$: Y_t is not a cause of X_{t+1}							H$_0$: X_t is not a cause of Y_{t+1}						
γ	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.0	0.1	0.2	0.3	0.4	0.5	0.6
HSNCIC	94	88	81	63	86	77	62	97	0	0	0	0	0	0
Granger	92	96	95	90	90	94	93	96	92	85	45	13	2	3

1-dimensional independent noise is added to $X(t)$ and $Y(t)$.

HSNCIC	97	96	93	85	81	68	75	96	0	0	0	0	0	0

Number of times accepting H$_0$ among 100 datasets (α = 5%)

Concluding Remarks

- Kernel dependence measures
  - The normalized (conditional) covariance on RKHS gives kernel-free measures of dependence in population.
  - The Gram matrix expression gives the p.d.-kernel estimate of the (conditional) mean square contingency.
  - Comparably reliable methods for conditional independence test.
- Future directions
  - More empirical studies
  - More theory on kernel choice
  - Application to causal inference (Sun et al., 2007).